isobar for developers

Florian P. Breitwieser, Jacques Colinge

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Contents

1 Introduction

This documents highlights the structure of the S4 classes and methods in the `isobar` pacakge.

```
>   library(isobar)
```

2 Classes

2.1 IBSpectra

```
>   getClass("IBSpectra")
```

```
Virtual Class "IBSpectra" [package "isobar"]

Slots:

Name:        proteinGroup   reporterTagNames  reporterTagMasses
Class:       ProteinGroup          character            numeric

Name:   isotopeImpurities                log          assayData
Class:              matrix             matrix          AssayData

Name:           phenoData        featureData     experimentData
Class: AnnotatedDataFrame AnnotatedDataFrame              MIAxE
```

```
Name:          annotation       protocolData  .__classVersion__
Class:          character AnnotatedDataFrame          Versions

Extends:
Class "eSet", directly
Class "VersionedBiobase", by class "eSet", distance 2
Class "Versioned", by class "eSet", distance 3

Known Subclasses:
Class "iTRAQSpectra", directly
Class "TMTSpectra", directly
Class "iTRAQ4plexSpectra", by class "iTRAQSpectra", distance 2
Class "iTRAQ8plexSpectra", by class "iTRAQSpectra", distance 2
Class "TMT2plexSpectra", by class "TMTSpectra", distance 2
Class "TMT6plexSpectra", by class "TMTSpectra", distance 2
Class "TMT6plexSpectra2", by class "TMTSpectra", distance 2
Class "TMT10plexSpectra", by class "TMTSpectra", distance 2
```

identifications and quantitative values. Spectrums are identified as stemming from distinct peptides, and quantitative information of each spectrum are extracted from a certain `m/z` region.

`IBSpectra` class holds this qualitative and quantitative information. It is a virtual class. It extends `eSet` from Biobase to store meta-information of spectrum identifications and quantitative information (`m/z` and `intensity`) of reporter tags. `eSet` is extended by slots for protein grouping, tag names, tag masses and isotope impurity correction matrix.

`ProteinGroup` objects store the mapping and grouping of peptide level identifications to protein identifications.

`IBSpectra` is a virtual class. Currently used isobaric tagging kits iTRAQ 4plex and 8plex, and TMT 2plex and 6plex are implemented in the `iTRAQ4plexSpectra`, `iTRAQ8plexSpectra`, `TMT2plexSpectra`, `TMT6plexSpectr` and `TMT10plexSpectr`, respectively. These are subclasses of `iTRAQSpectra` and `TMTSpectra`, resp. which in turn are virtual subclasses of `IBSpectra`.

2.2 ProteinGroup

```
> getClass("ProteinGroup")

Class "ProteinGroup" [package "isobar"]

Slots:

Name:          spectrumToPeptide                spectrumId
Class:                  character                data.frame

Name:         peptideSpecificity           peptideNProtein
Class:                 data.frame                    matrix
```

```
Name:  indistinguishableProteins         proteinGroupTable
Class:                 character                data.frame

Name:        overlappingProteins      isoformToGeneProduct
Class:                     matrix                data.frame

Name:                proteinInfo               peptideInfo
Class:                 data.frame                data.frame

Name:          .__classVersion__
Class:                   Versions

Extends:
Class "VersionedBiobase", directly
Class "Versioned", by class "VersionedBiobase", distance 2
```

mapped back to proteins. This mapping leads to protein groups, which explain the observed peptides according to the parsimony law.

A `ProteinGroup` object is generated when a `IBSpectra` object is created by `readIBSpectra`. Protein to peptide to spectrum mapping is extracted from a suitable identication format[1]

2.3 NoiseModel

```
>   getClass("NoiseModel")

Virtual Class "NoiseModel" [package "isobar"]

Slots:

Name:          na.region     low.intensity                 f         parameter
Class:           numeric           numeric          function           numeric

Name:  .__classVersion__
Class:          Versions

Extends:
Class "VersionedBiobase", directly
Class "Versioned", by class "VersionedBiobase", distance 2

Known Subclasses: "ExponentialNoANoiseModel", "ExponentialNoiseModel", "InverseNoi
"InverseNoANoiseModel", "GeneralNoiseModel"
```

in the spectrum-level ratios of a certain experimental setup.

[1] IBSpectra CSV, and MzIdentML format. Mascot DAT and Phenyx pidres.xml format converters to IBSpectra format are provided.

3 Session Information

The version number of R and packages loaded for generating the vignette were:

- R version 4.4.1 (2024-06-14), `x86_64-pc-linux-gnu`
- Locale: `LC_CTYPE=en_US.UTF-8`, `LC_NUMERIC=C`, `LC_TIME=en_US.UTF-8`, `LC_COLLATE=C`, `LC_MONETARY=en_US.UTF-8`, `LC_MESSAGES=en_US.UTF-8`, `LC_PAPER=en_US.UTF-8`, `LC_NAME=C`, `LC_ADDRESS=C`, `LC_TELEPHONE=C`, `LC_MEASUREMENT=en_US.UTF-8`, `LC_IDENTIFICATION=C`
- Time zone: `Etc/UTC`
- TZcode source: `system (glibc)`
- Running under: `Ubuntu 24.04 LTS`
- Matrix products: default
- BLAS: `/usr/lib/x86_64-linux-gnu/openblas-pthread/libblas.so.3`
- LAPACK: `/usr/lib/x86_64-linux-gnu/openblas-pthread/libopenblasp-r0.3.26.so` ; LAPACK version3.12.0
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: Biobase 2.65.0, BiocGenerics 0.51.0, isobar 1.51.0
- Loaded via a namespace (and not attached): AnnotationDbi 1.67.0, BiocFileCache 2.13.0, Biostrings 2.73.1, DBI 1.2.3, GenomeInfoDb 1.41.1, GenomeInfoDbData 1.2.12, IRanges 2.39.0, KEGGREST 1.45.1, MASS 7.3-61, R6 2.5.1, RSQLite 2.3.7, Rcpp 1.0.12, S4Vectors 0.43.0, UCSC.utils 1.1.0, XVector 0.45.0, biomaRt 2.61.2, bit 4.0.5, bit64 4.0.5, blob 1.2.4, buildtools 1.0.0, cachem 1.1.0, cli 3.6.3, colorspace 2.1-0, compiler 4.4.1, crayon 1.5.3, curl 5.2.1, dbplyr 2.5.0, digest 0.6.36, distr 2.9.3, dplyr 1.1.4, fansi 1.0.6, fastmap 1.2.0, filelock 1.0.3, generics 0.1.3, ggplot2 3.5.1, glue 1.7.0, grid 4.4.1, gtable 0.3.5, hms 1.1.3, httr 1.4.7, httr2 1.0.1, jsonlite 1.8.8, knitr 1.47, lifecycle 1.0.4, magrittr 2.0.3, maketools 1.3.0, memoise 2.0.1, munsell 0.5.1, pillar 1.9.0, pkgconfig 2.0.3, plyr 1.8.9, png 0.1-8, prettyunits 1.2.0, progress 1.2.3, rappdirs 0.3.3, rlang 1.1.4, scales 1.3.0, sfsmisc 1.1-18, startupmsg 0.9.6.1, stats4 4.4.1, stringi 1.8.4, stringr 1.5.1, sys 3.4.2, tibble 3.2.1, tidyselect 1.2.1, tools 4.4.1, utf8 1.2.4, vctrs 0.6.5, xfun 0.45, xml2 1.3.6, zlibbioc 1.51.1